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SUPERLATTICE PRESENCE IN Cu_3Au AND FeCo SYSTEMS

by

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X-ray diffraction techniques have been widely used in establishing the presence of superlattice structures for alloy systems. In a superlattice structure the two atoms of a binary alloy occupy definite positions with respect to atoms of the companion species, in contrast to the usual random substitutional location of one atom in the structure of the other. For instance, in disordered Cu_3Au, the gold atoms are arrayed randomly at sites normally occupied by copper atoms in the copper lattice, but in ordered Cu_3Au all of the gold atoms are located at cube corners and copper atoms at face-centered positions of the unit-cell cube. Transformations from one state into the other can be invoked by suitable thermal treatment. The diffraction patterns for the two states will differ markedly depending upon the degree of ordering and the relative scattering power of the individual atomic species. Many systems such as CuZn, FeCo, etc., are difficult to study with x-rays since the scattering amplitudes for x-rays of the two atoms are so similar in value. It seemed of interest to study such systems by neutron diffraction where the scattering amplitudes might be more favorable.

Cu_3Au was selected for initial study since superstructure effects are very pronounced for this alloy as shown by extensive investigations with X-ray diffraction, resistivity measurement, etc. techniques.

When the neutron study was started, neither the gold coherent scattering cross section nor phase of scattering was known, so it was anticipated that information on these would be obtained from the alloy study. Figure 1 shows the neutron diffraction powder patterns which were obtained for samples of the ordered and disordered alloy. X-ray diffraction measurements by Dr. M. A. Bredig of the Chemistry Division showed pronounced superstructure in the ordered sample as evidenced by the presence of diffraction peaks at the (100), (110), (210), (211), etc., positions in contrast to their absence in the disordered sample.

The neutron diffraction patterns, however, are seen to be indistinguishable with unmeasurably small scattering at the positions indicated for superstructure scattering. Since the intensity of the superstructure lines is proportional to $(f_{Au} - f_{Cu})^2$, it is concluded that the two amplitudes for neutron scattering are close in value and of the same sign.

Values for f_{Au} can be obtained from the intensities of the (111) and (200) peaks for both the ordered and disordered specimens. The structure factor for these peaks is $(3\, f_{Cu} + f_{Au})$ and using the independently obtained value of $f_{Cu} = 0.77 \times 10^{-12}$ cm, one obtains $f_{Au} = 0.90 \times 10^{-12}$ cm so that the coherent scattering cross section for gold is given as 10 barns. This value is subject to an uncertainty of about 2 barns and compares not unfavorably with the value of 7 barns obtained recently from the direct measurement of the weak peaks in the pattern for pure gold. In any event, a scattering cross section for gold of 7 to 10 barns with a positive scattering amplitude accounts satisfactorily for the observed absence of superstructure lines in the ordered Cu_3Au pattern.

Samples of ordered and disordered FeCo have been examined in the same fashion as Cu_3Au. For this case, conventional x-ray analysis breaks down because of the similarity of the scattering centers, but indirect measurements of electrical resistivity suggest strongly the presence of superstructure.

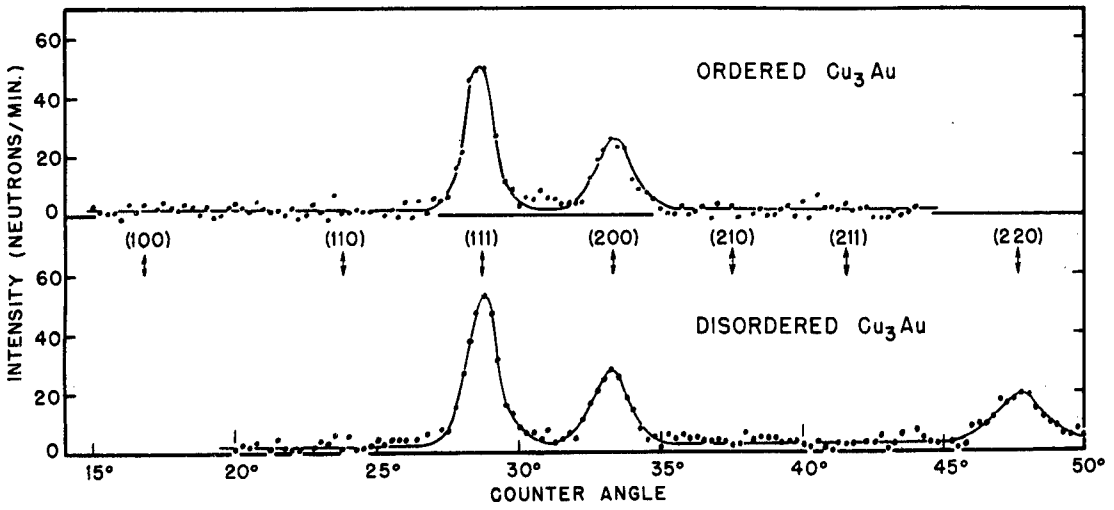

Figure 1.

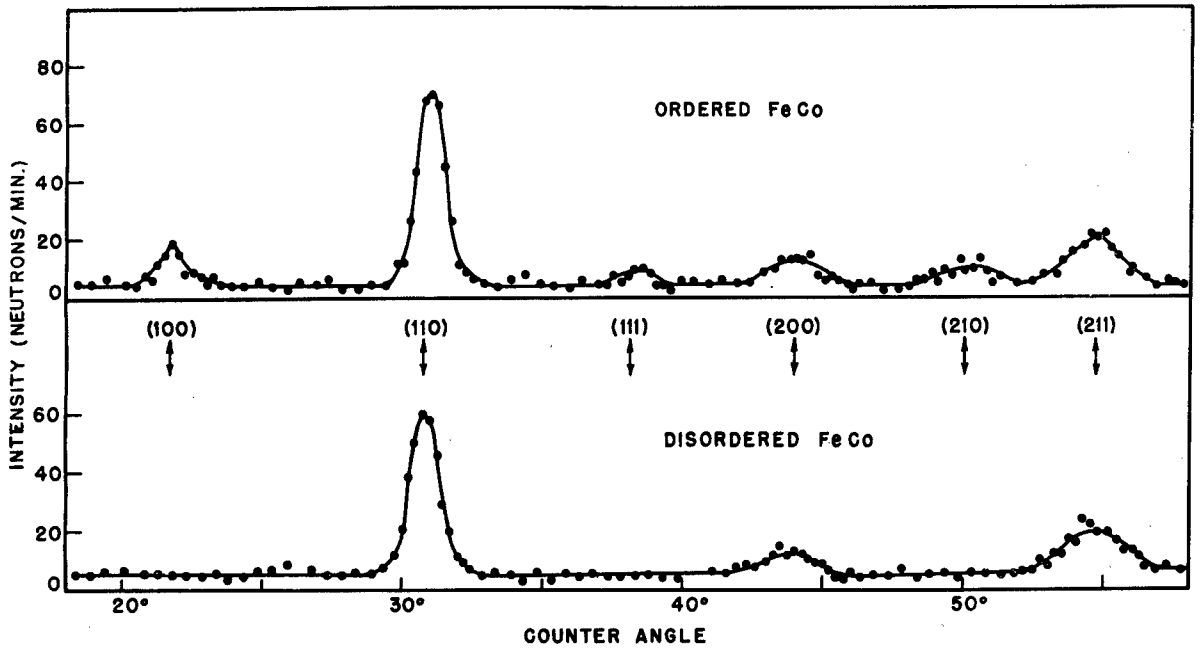

Figure 2.

The coherent scattering cross sections for neutrons of Fe and Co are markedly different, being 13 and 1.5 barns, respectively, so that measurable differences should be obtained. Figure 2 shows the neutron diffraction patterns obtained for ordered and disordered preparations and the appearances of the superstructure lines for the ordered preparation at (100), (111), and (210) positions is to be noted. The pattern for the ordered sample is similar to the CaCl-type pattern so that iron atoms are located at the corners of a simple cube and cobalt atoms at the body-centered positions of the cube. If the scattering amplitudes of Fe and Co obtained from other materials are used for calculating the expected intensity of the superstructure lines, one finds good agreement with the measured values. This indicates that the degree of ordering is quite high, being in the region of 90 to 100 per cent.

Similar measurements have been started for samples of Ni_3Mn. This system should prove interesting since Mn possesses a negative scattering amplitude compared to the positive amplitude of Ni and hence the diffraction effects characteristic of superstructure should be enhanced.

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